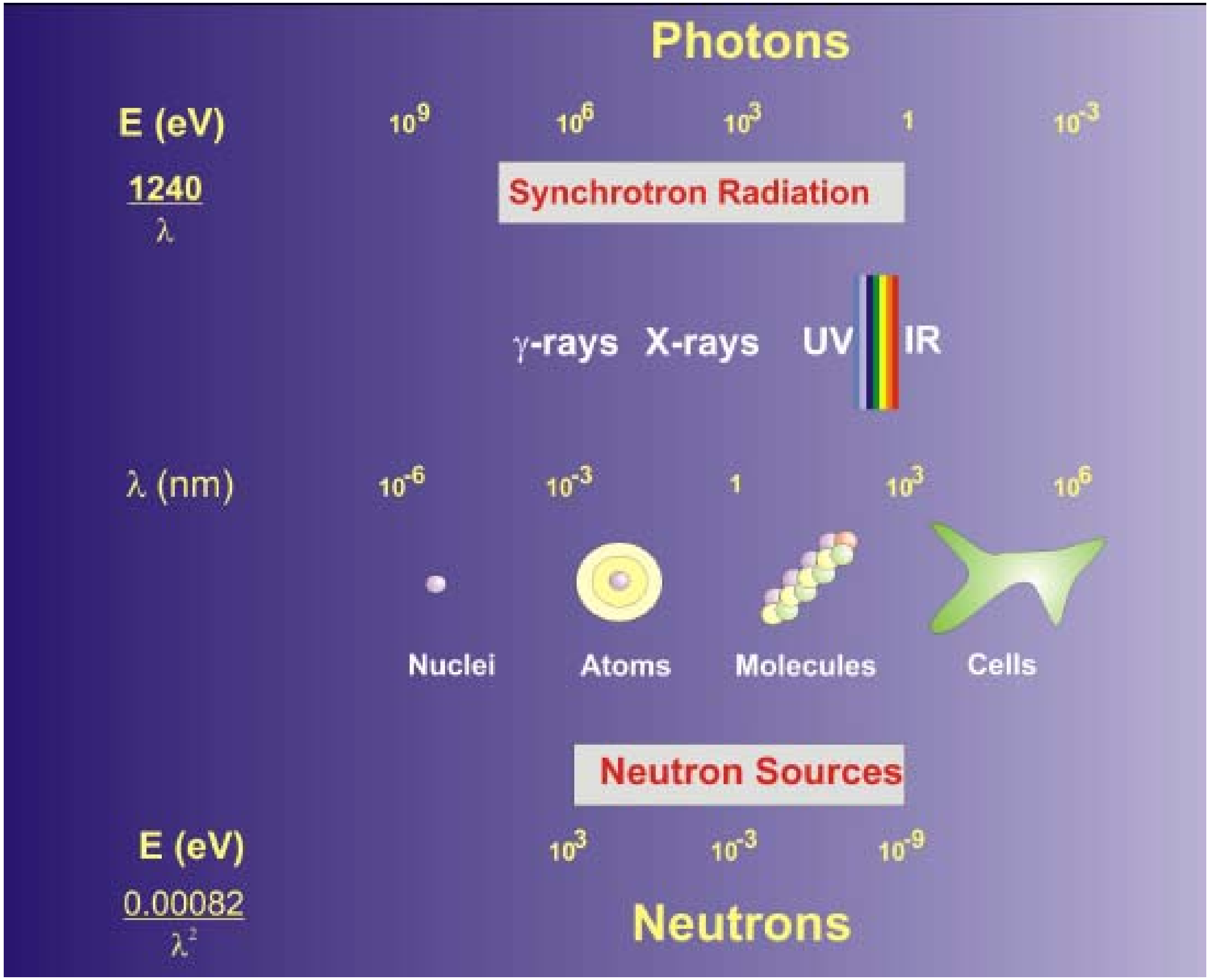
Tenth National School on Neutron and X-ray Scattering

Argonne NATIONAL LABORATORY

OAK RIDGE National Laboratory

Why Neutron and X-ray?



X-ray

0.1-10 Å

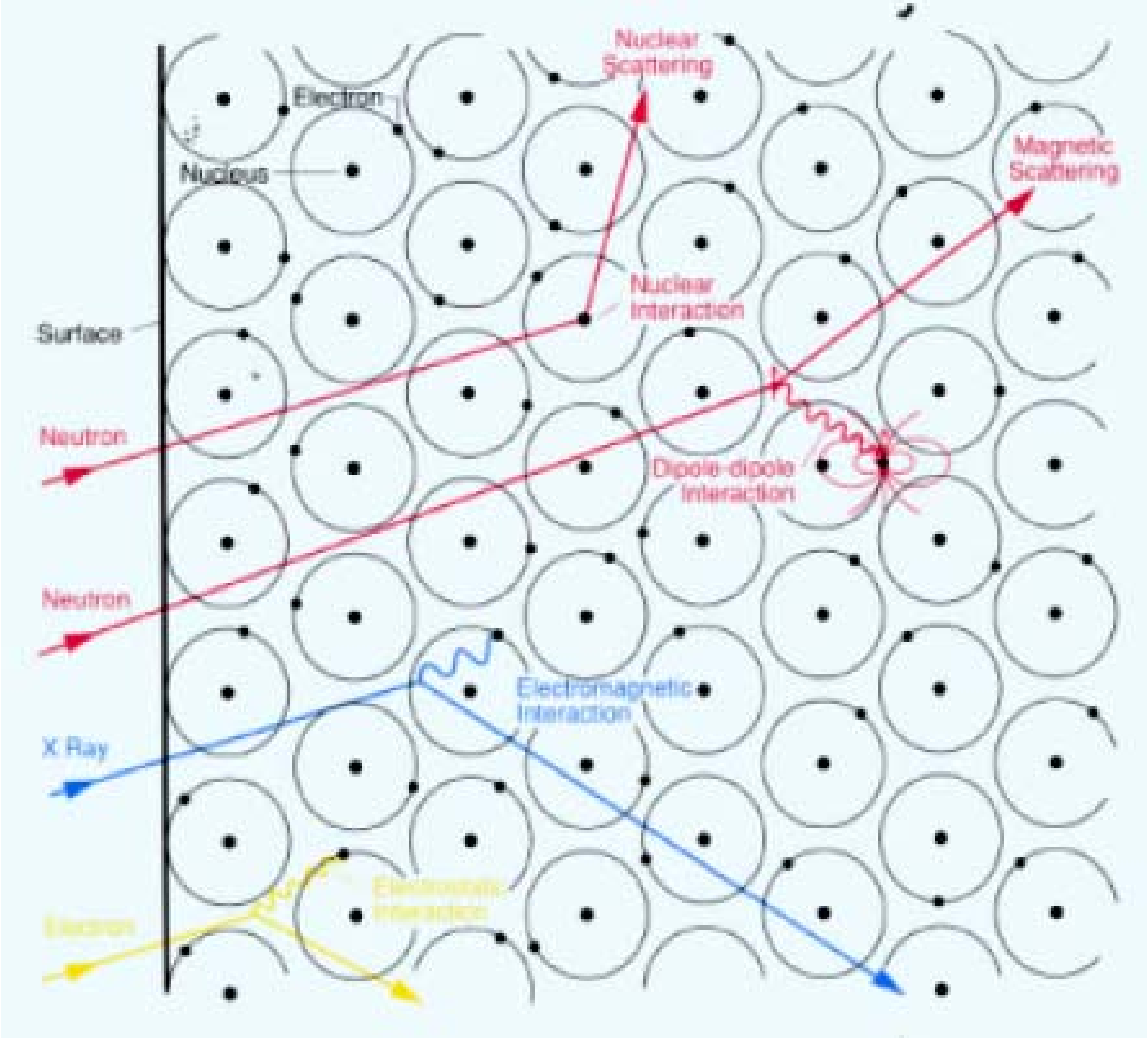
1-100 keV

Neutron

0.3-3 Å

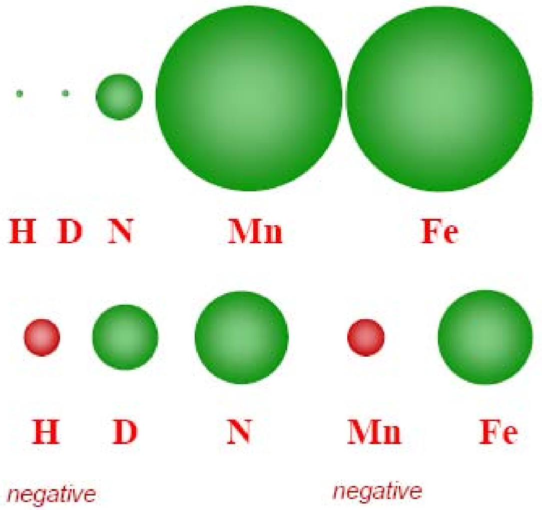
0.1-1000meV

Interaction of Neutron and X-ray with Matter



Neutron vs. X-ray

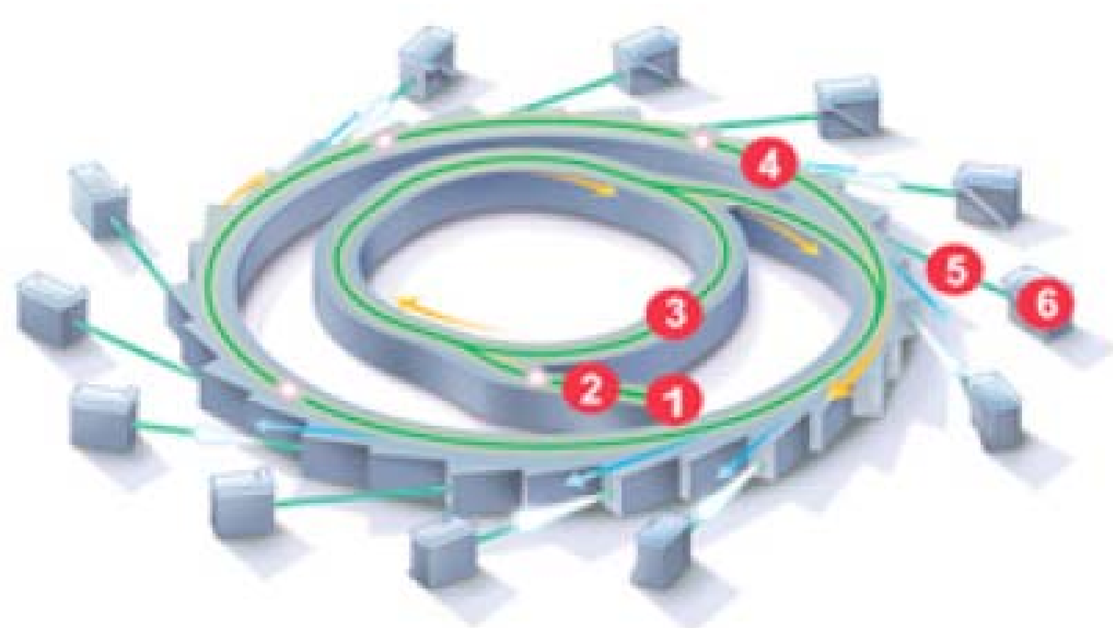
X-ray scattering length



Neutron scattering length

- **Synchrotron X-rays**
  - High throughput
  - Time-resolution (ms)
  - Tunable energy (ASAXS)
  - Micro & nanofocused beams for scanning (diffraction, imaging)
  - Ultrathin films (GISAXS)
- **Neutrons**
  - Sensitive to light atoms: polymers, biology, soft condensed matter, hydrogen in metals
  - Isotope labeling (Multi-component systems)
  - No radiation damage
  - High penetration
    - bulky specimens
    - complicated environments (P,T)
  - Magnetic contrast

How do we produce X-rays?



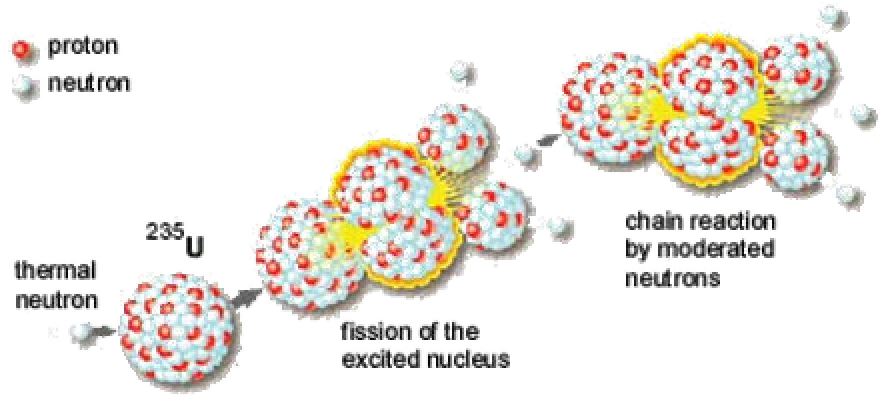
1. Electron gun
2. Linear Accelerator LINAC
3. Booster Synchrotron
4. Storage Ring (SR)
5. Beamline
6. Experiment station

(Courtesy: Australian Synchrotron, Illustrator: Michael Payne)

Argonne APS Facility

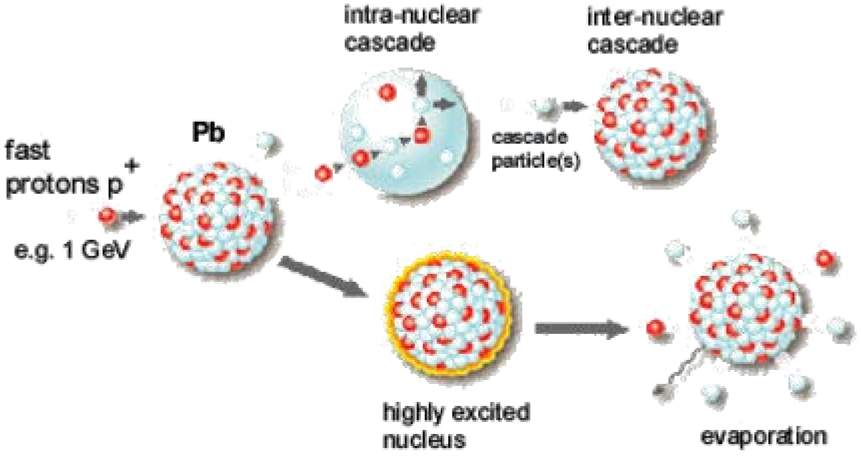
The Advanced Photon Source Accelerator Complex

How do we produce neutrons?



Fission

- Chain reaction
- Continuous flow
- ~ 1 neutron/fission

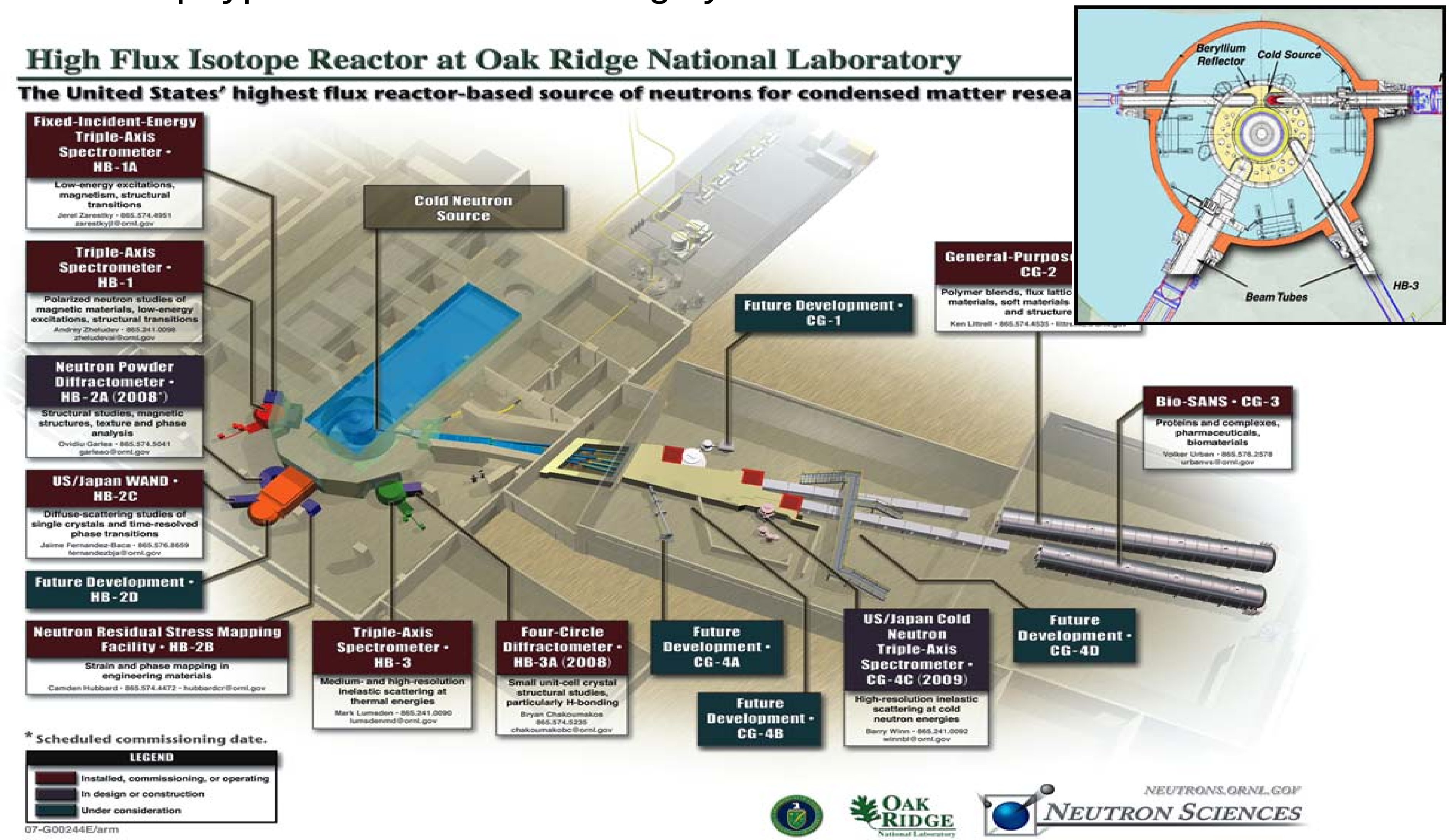


Spallation

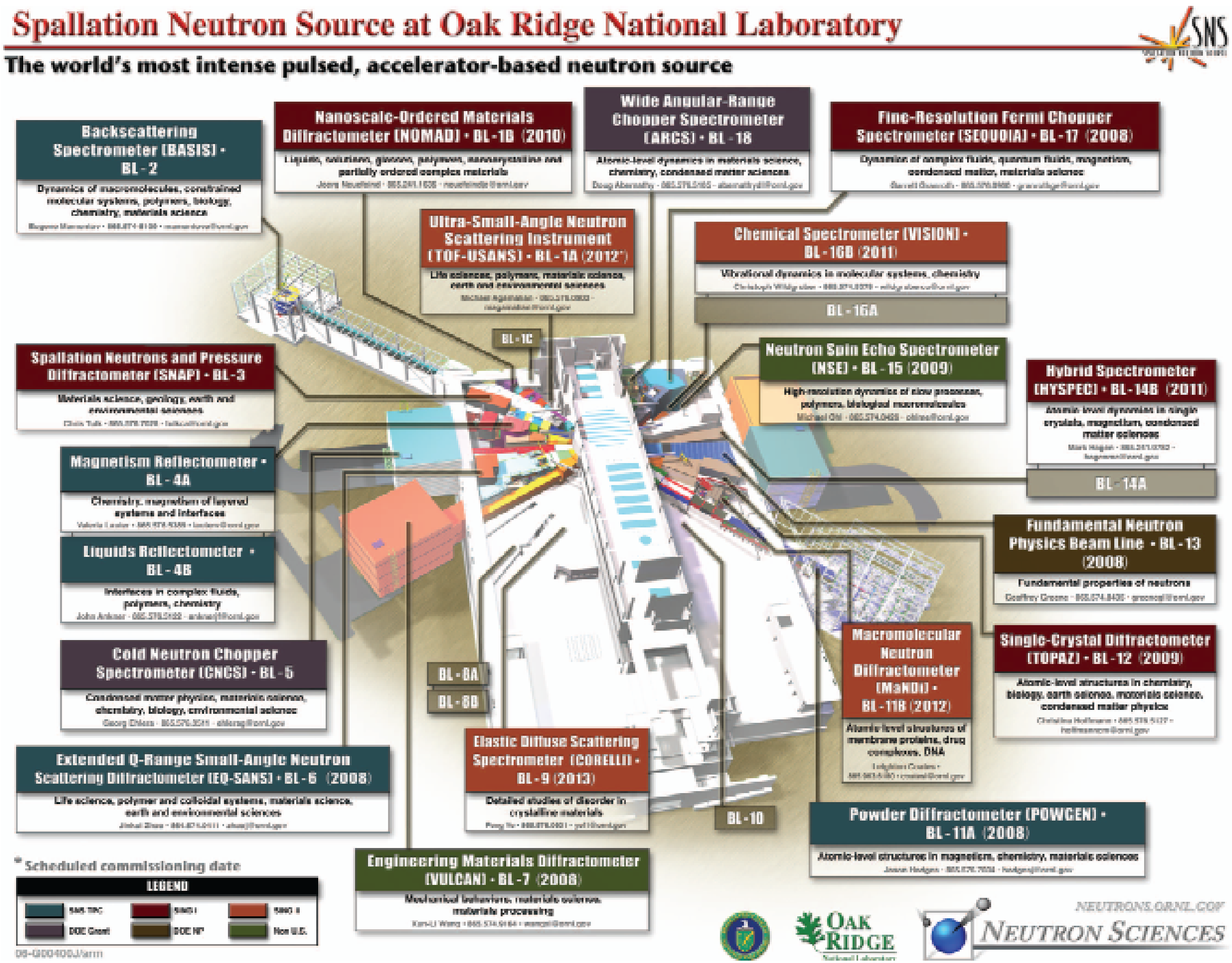
- No chain reaction
- Accelerator driven
- Pulsed operation
- ~ 30 neutrons/proton

Oak Ridge Facility ----HFIR

The HFIR is a beryllium-reflected, light-water-cooled and -moderated, flux-trap type reactor that uses highly enriched uranium-235 as the fuel.



Oak Ridge Facility--SNS



Experiments

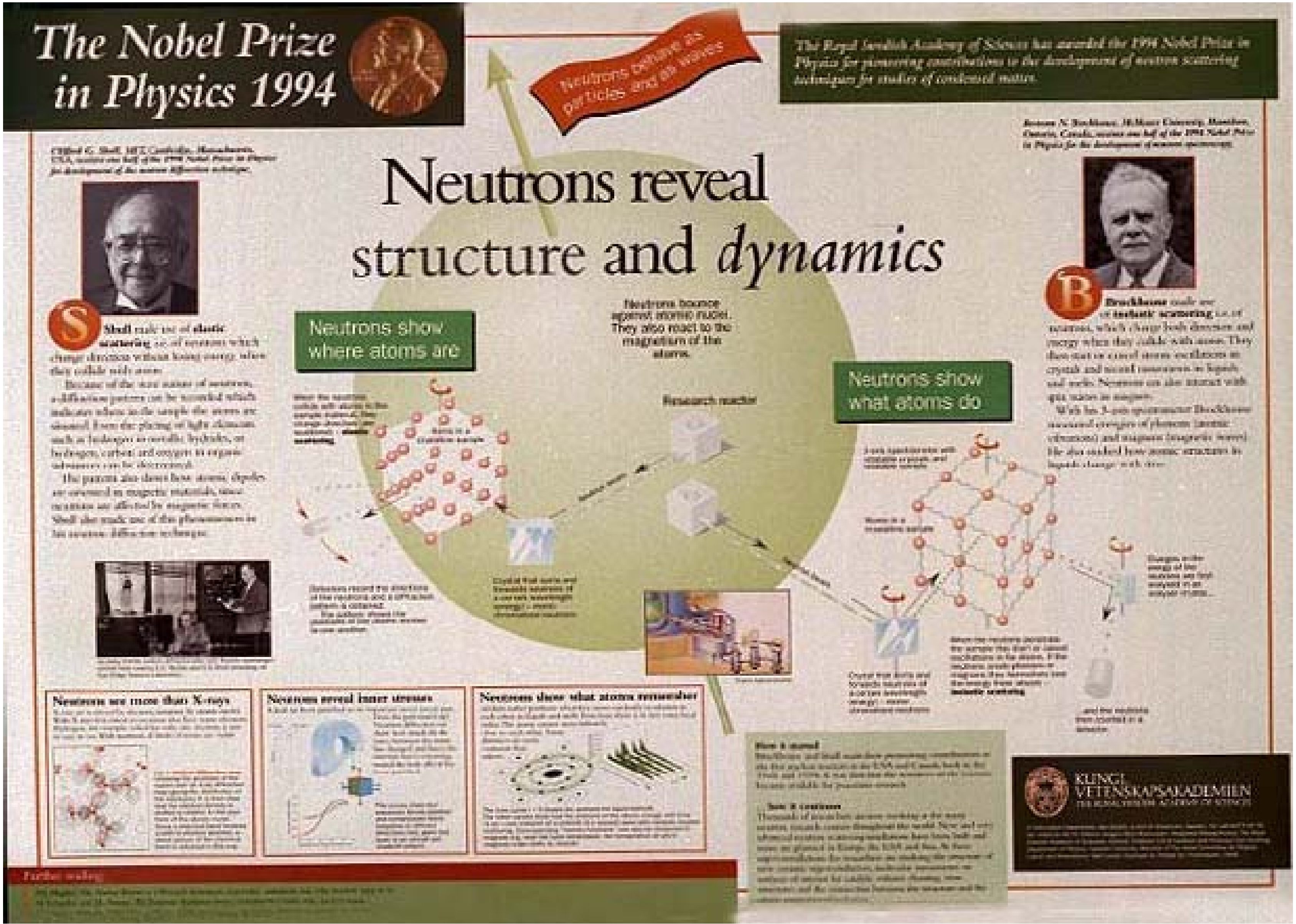
Neutron:

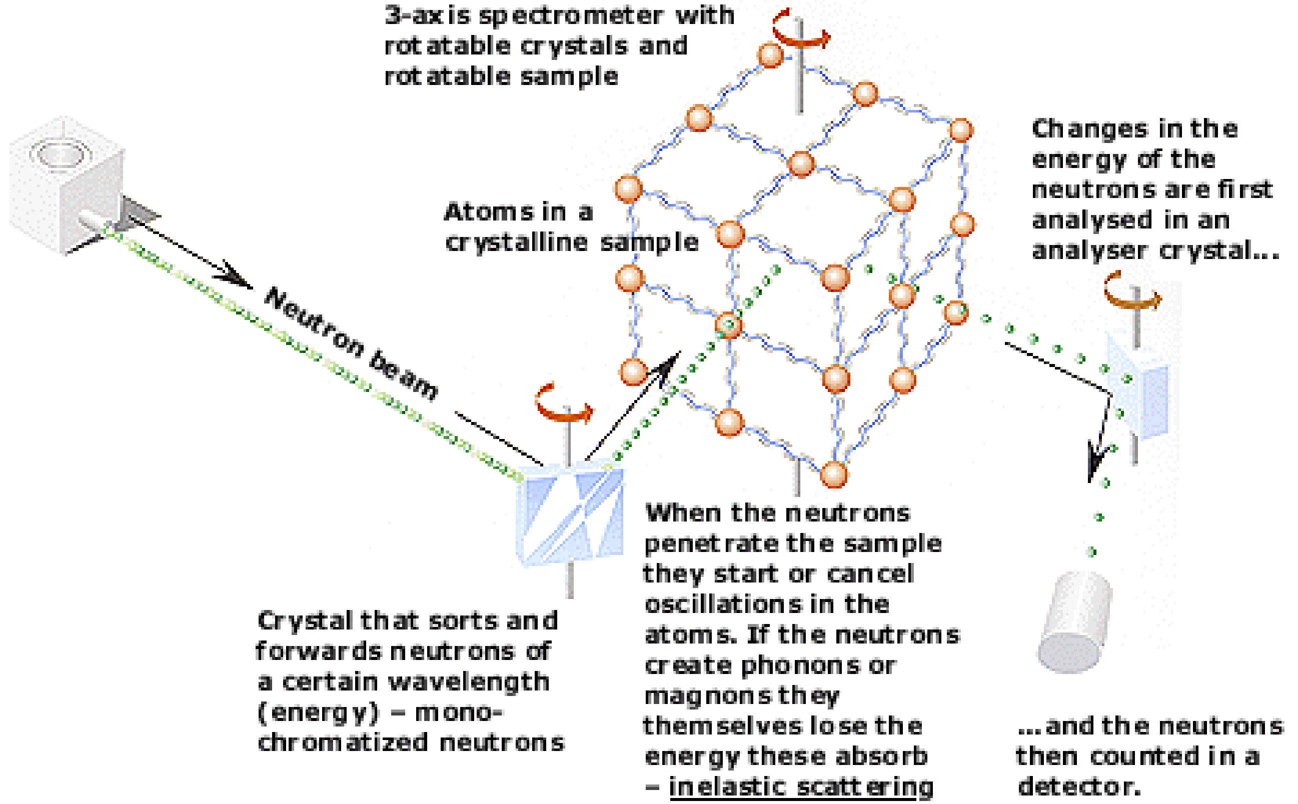
- Triple Axis Spectrometer
- Small Angle Neutron Scattering(SANS)
- Wide Angular-Range Chopper Spectrometer (ARCS)

X-Ray:

- Small Angle X-ray Scattering(SAXS)
- High Pressure Powder Diffraction
- X-ray Computed Micro-Tomography(XCMT)

Triple-axis Spectrometer





Momentum transfer

$$Q = k_i - k_f$$

Energy transfer

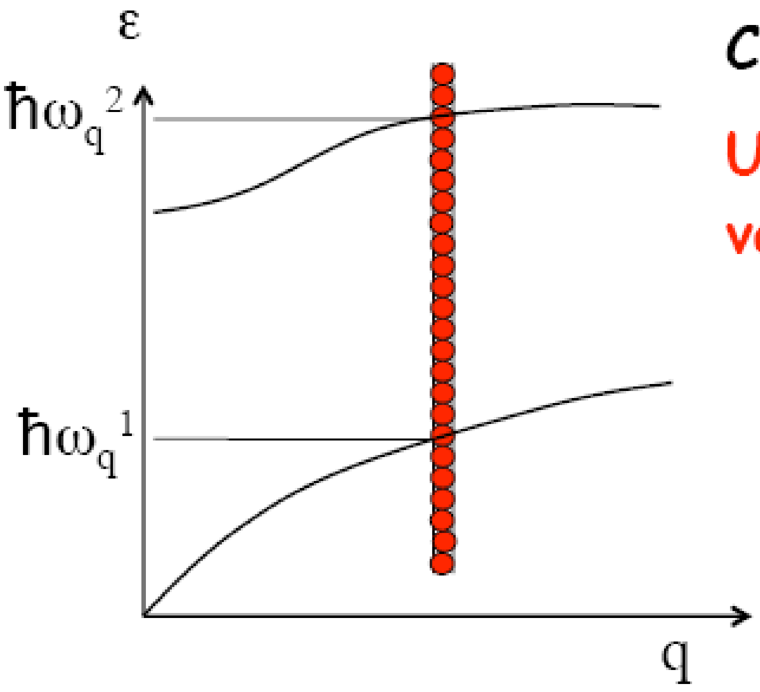
$$E = \hbar\omega = \hbar k_i^2/2m - \hbar k_f^2/2m$$

Inelastic scattering

$\hbar\omega > 0$ "Energy loss"

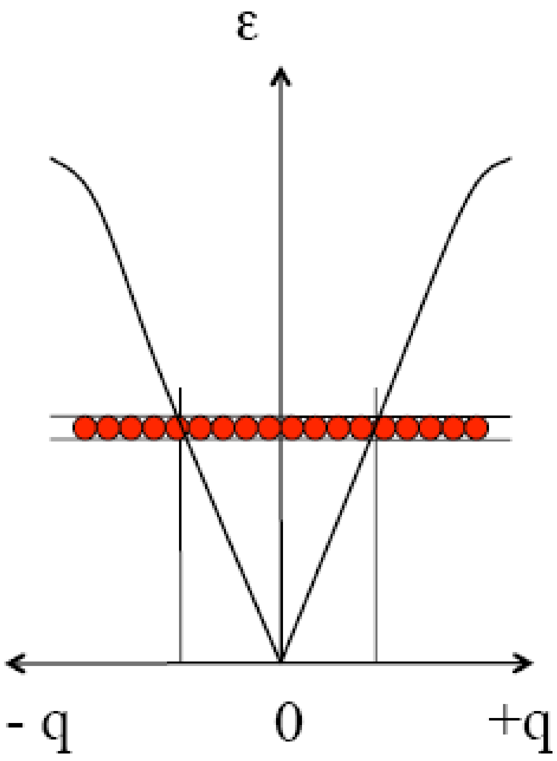
$\hbar\omega < 0$ "Energy gain"

Constant Q and Constant ε Scans



Constant Q scan

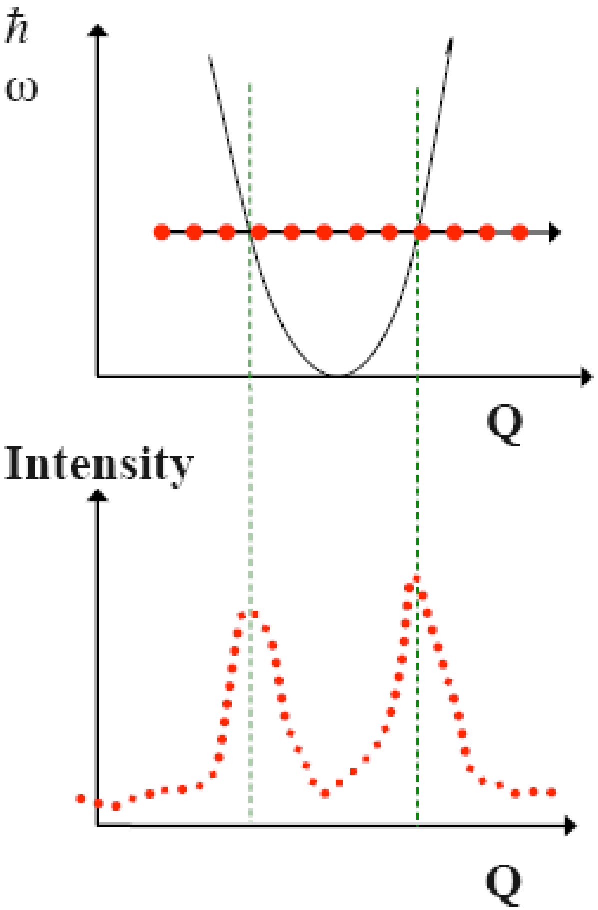
Used to measure slowly varying dispersion relations.

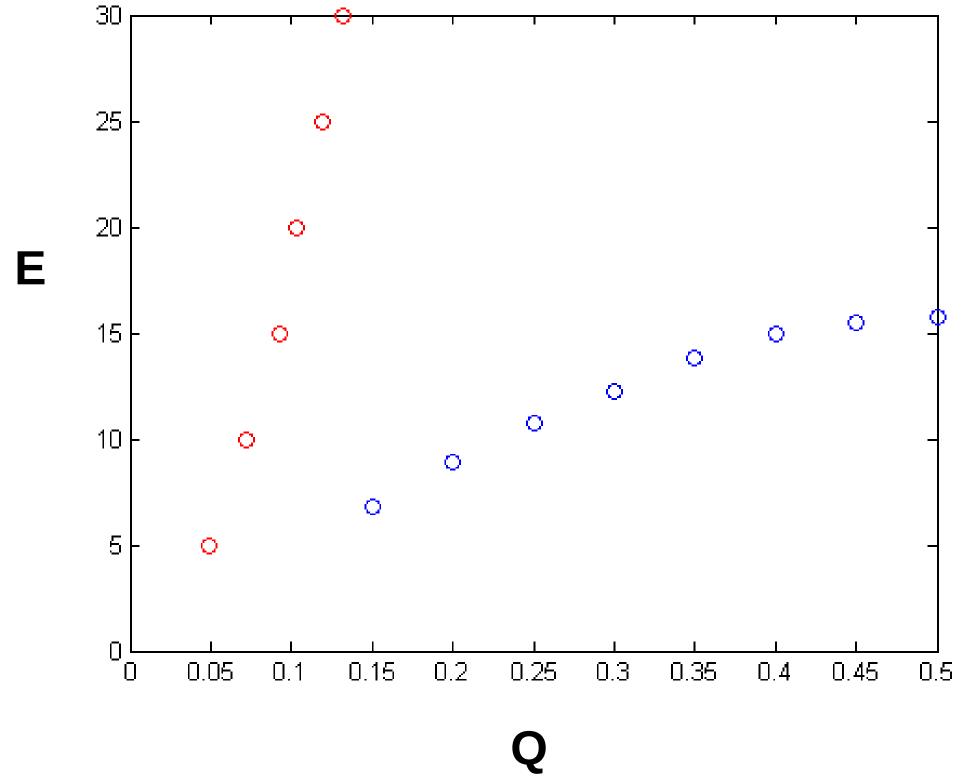


Constant ε scan

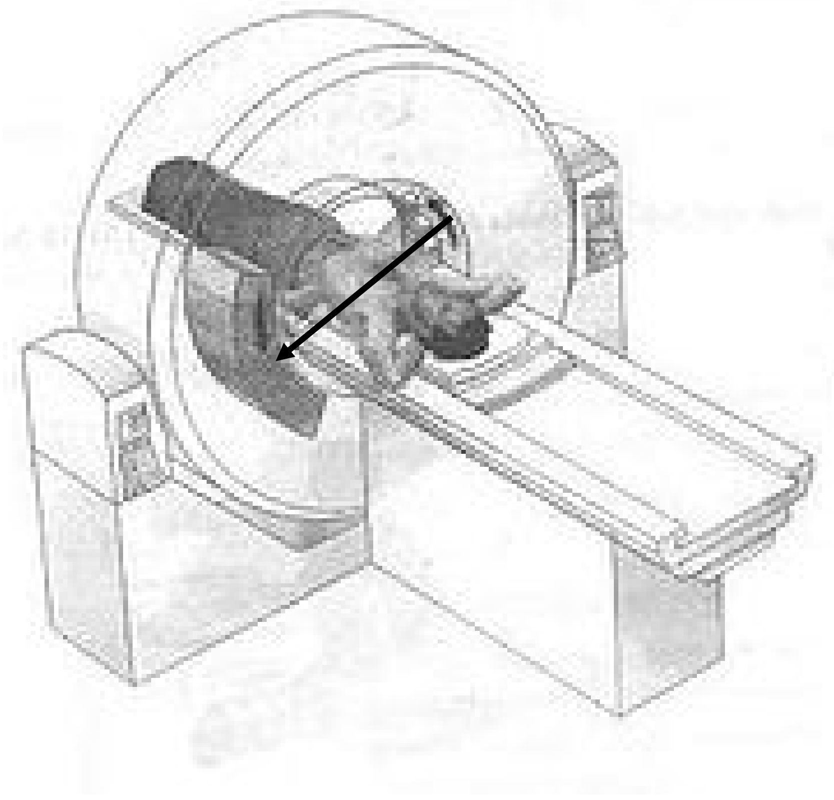
Used to measure steep Dispersion relations.

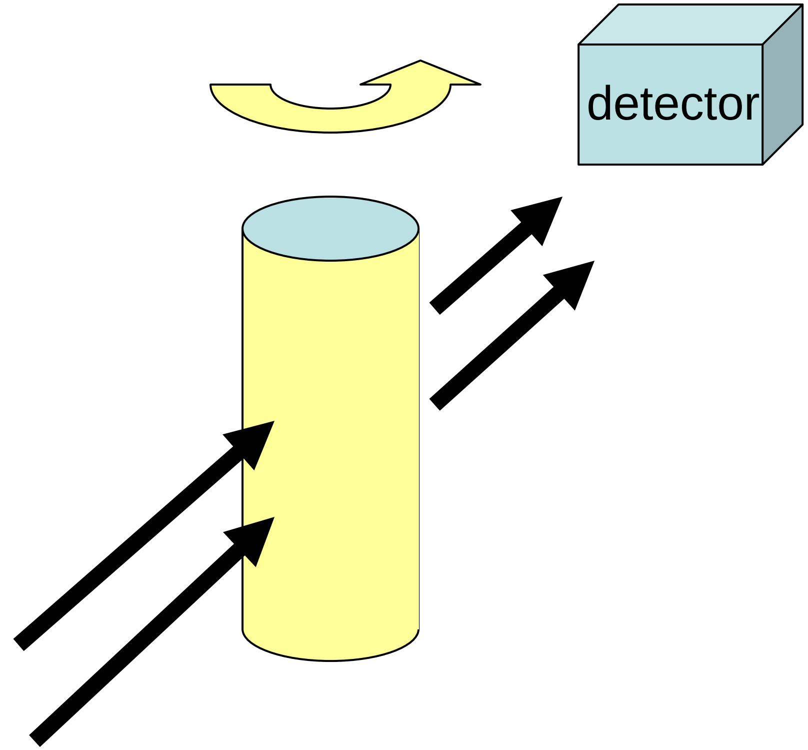
Dispersion Relation of Fe-Ga Alloy





Computed X-ray Micro-Tomography ----CMT



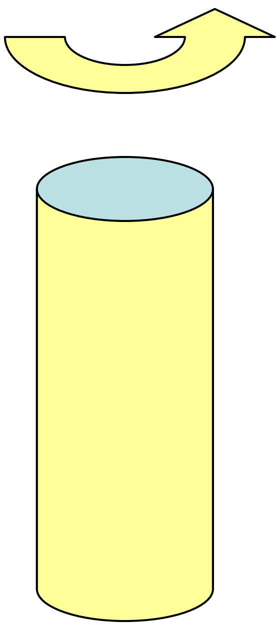


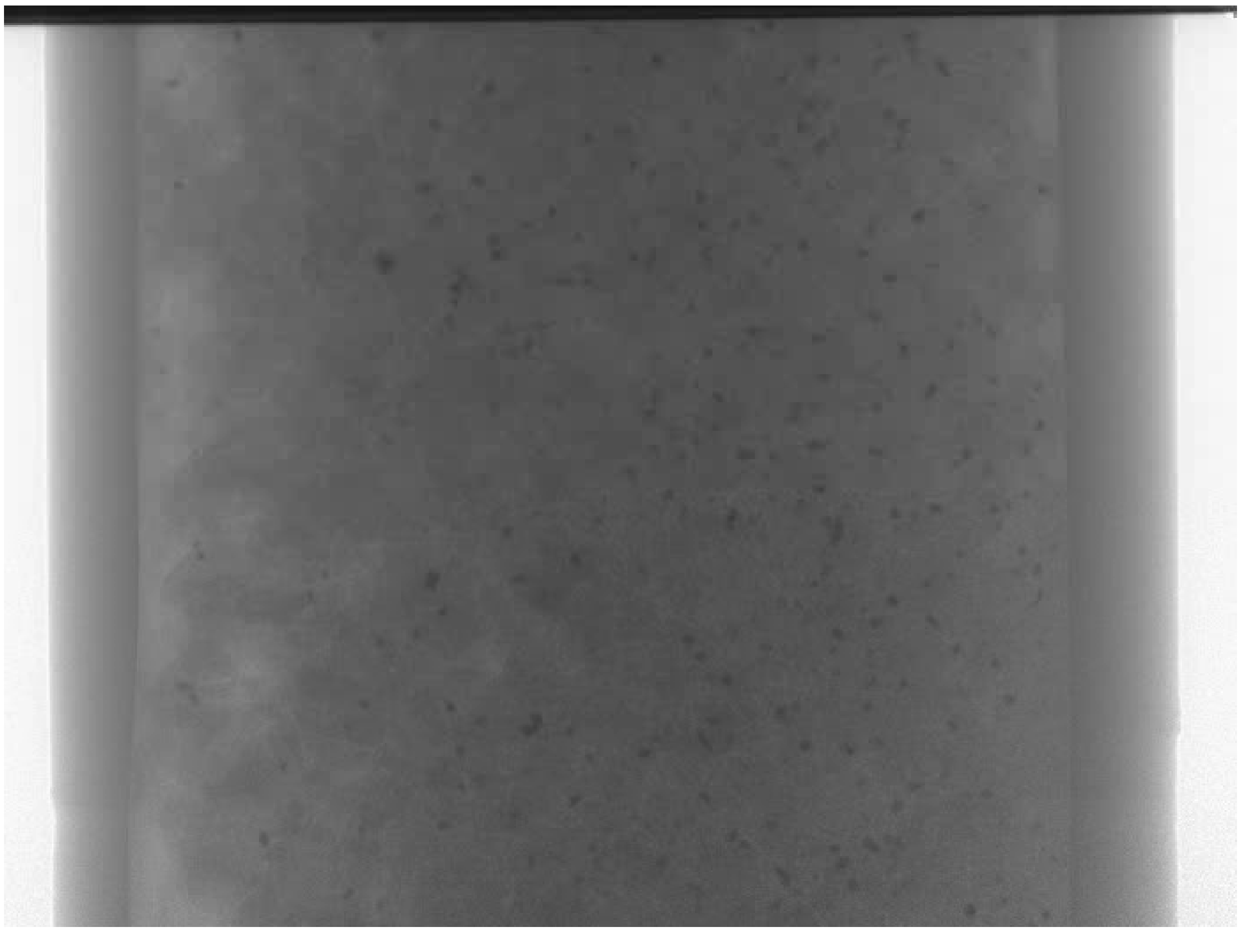
Medical Imaging CT
0.5-1mm resolution

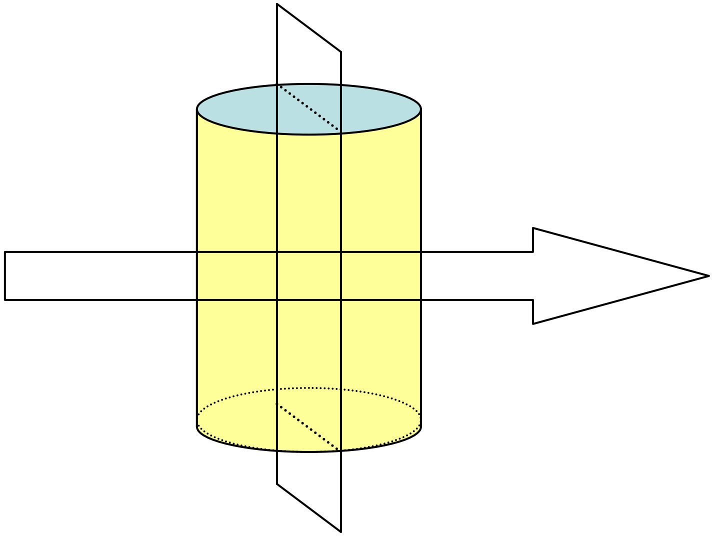
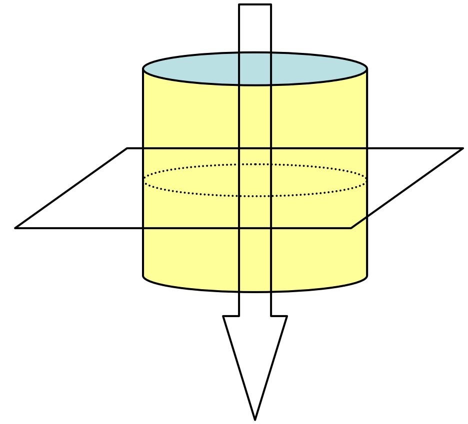
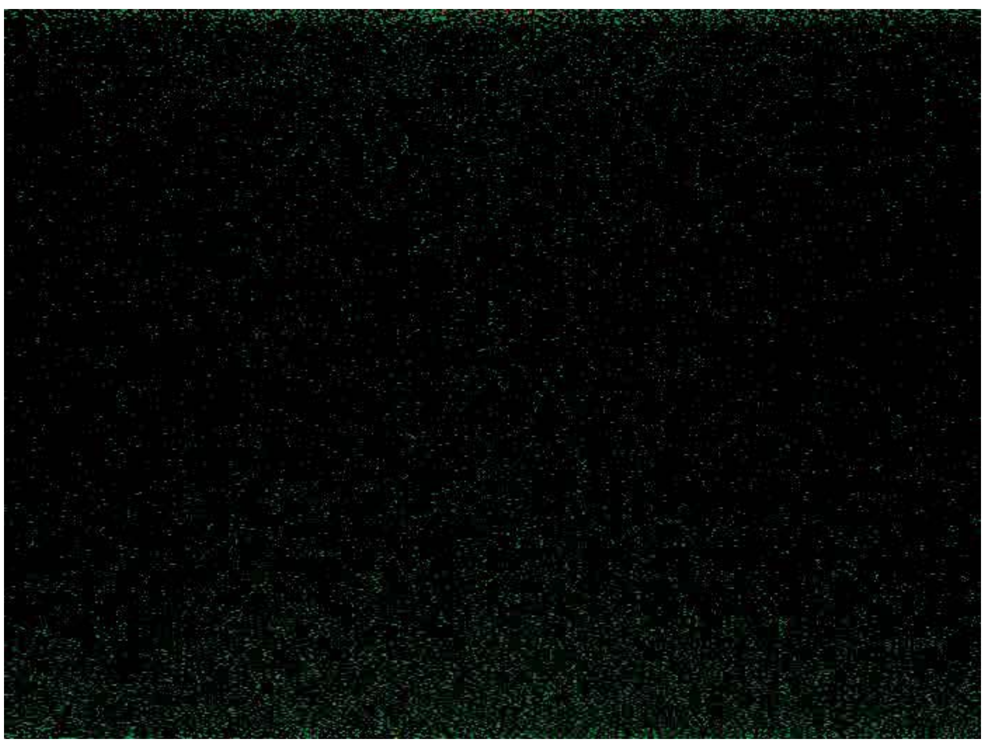
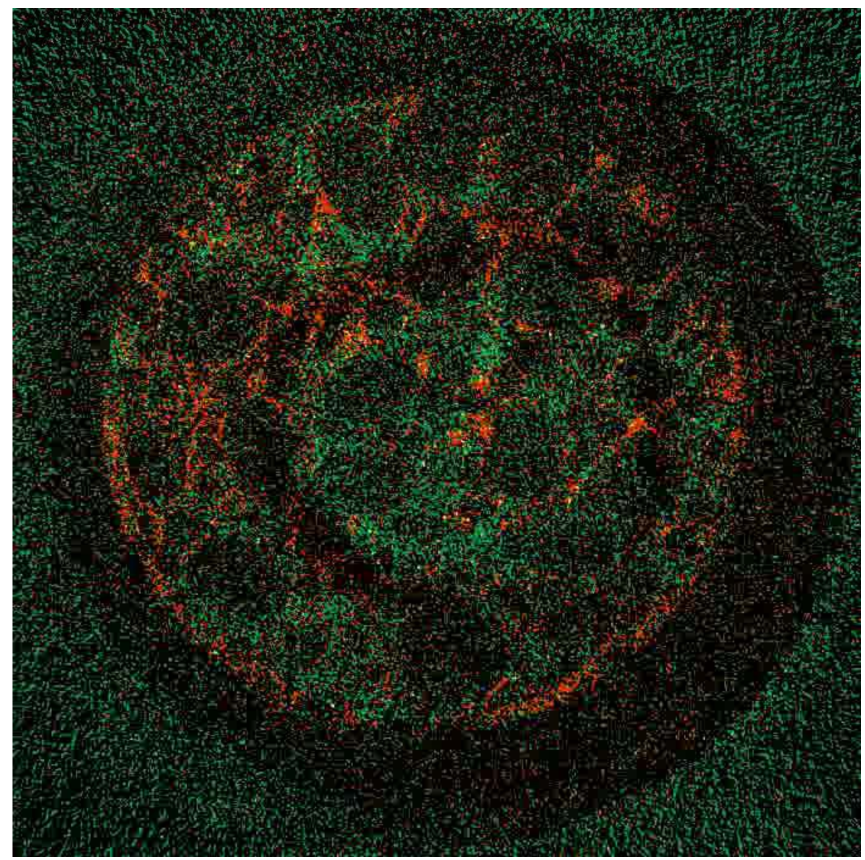
Micro-CT
Down to 1 micro

- Sample: a soil that contains water,solid and oil
- Goal: to image the distribution of two liquids in soil
- Contrast: enhance the contrast by doping water with cesium(Cs) and doping the oil with iodine (I).
- Energies:100eV above and below the I K absorption edge (33.139 keV) and 100ev above and below the Cs K absorption edge (36.985keV)
- measuring the transmitted x-ray image as the sample is rotated 180 degrees in 0.25 degree steps

- data → normalization → reconstruction(FFT tech) → 3-D cross-sections





Thank you!

The Advanced Photon Source Accelerator Complex

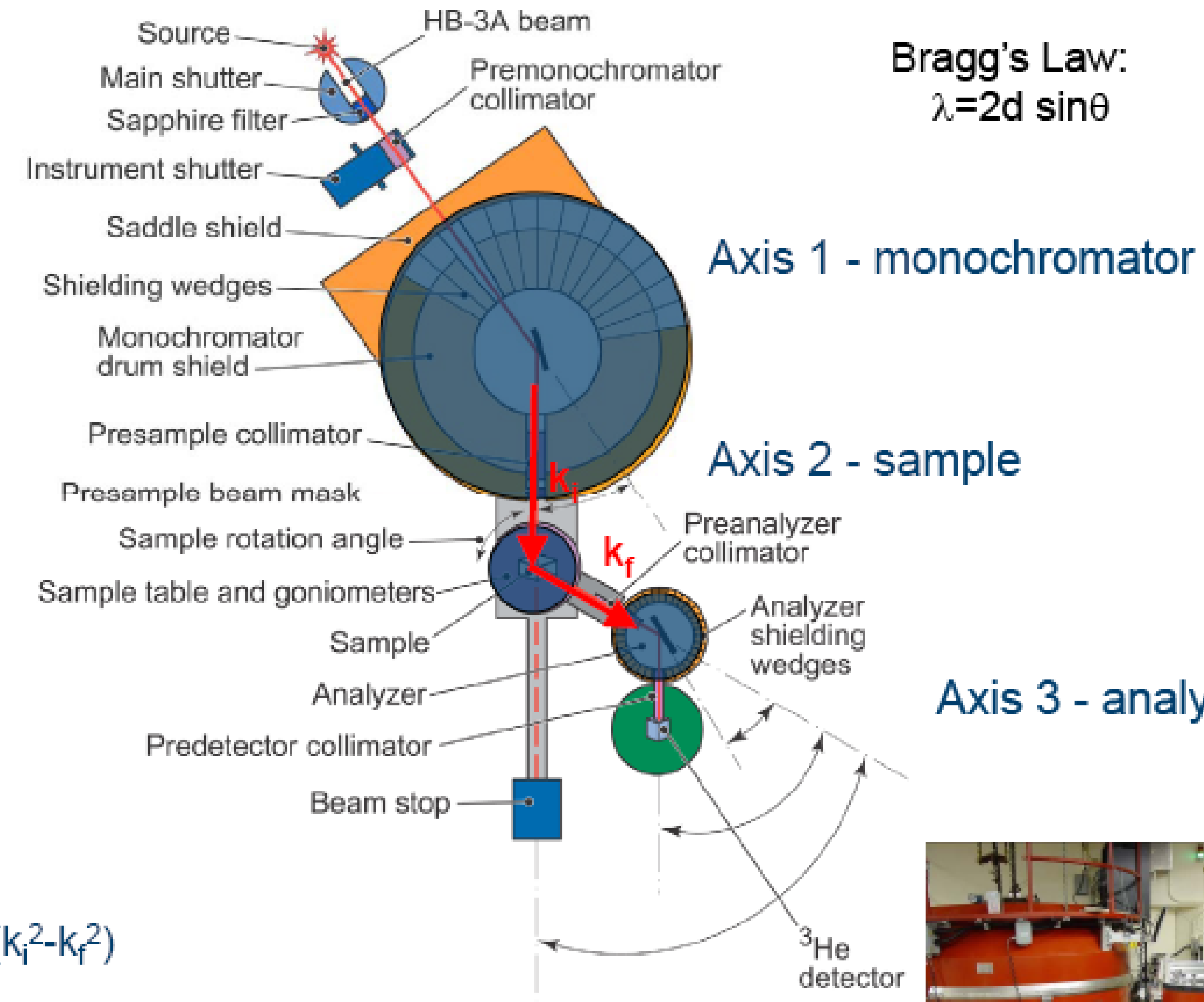
NXschool Lectures

- **Interaction of X-rays and Neutrons with Matter -- D. F. McMorrow**
- **Real/Reciprocal Space/Complementarity -- J. M. Gibson**
- **Powder Diffraction -- J. J. Rhyne**
- **Reflectivity/Magnetic Scattering -- C. F. Majkrzak**
- **Single Crystal Diffraction -- X. Wang**
- **Diffuse Scattering/Micro-Diffraction -- G. E. Ice**
- **Powder Diffraction Applications -- A. Huq**
- **PDF Analysis -- T. E. Proffen**
- **Small Angle Scattering -- S. Krueger**
- **High-Pressure Techniques -- W. Mao**
- **Magnetic Spectroscopy and Scattering -- E. Fullerton**
- **Neutron and X-rays for NanoScience -- E. D. Isaacs**

- **X-ray Generation/Instrumentation -- D. M. Mills**
- **X-ray Detection/Sources -- S. M. Gruner**
- **Synchrotron Sources -- P. Zschack**
- **X-ray Absorption Fine Structure (XAFS) -- G. B. Bunker**
- **Coherent X-ray Scattering -- L. B. Lurio**
- **Inelastic X-ray Scattering -- P. M. Abbamonte**
- **X-ray Imaging -- S. R. Stock**
- **Time-Resolved X-ray Scattering -- D. A. Reis**

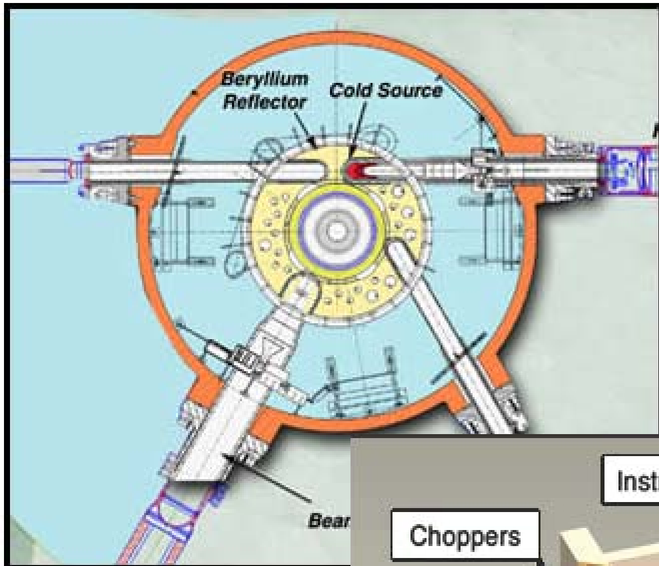
- **Neutron Generation/Detection -- J. M. Carpenter**
- **Neutron Sources -- J. J. Rhyne**
- **Quasi-elastic Neutron Scattering -- K. W. Herwig**
- **Inelastic Neutron Scattering -- R. Osborn**
- **Spin-Echo Techniques -- R. Pynn**

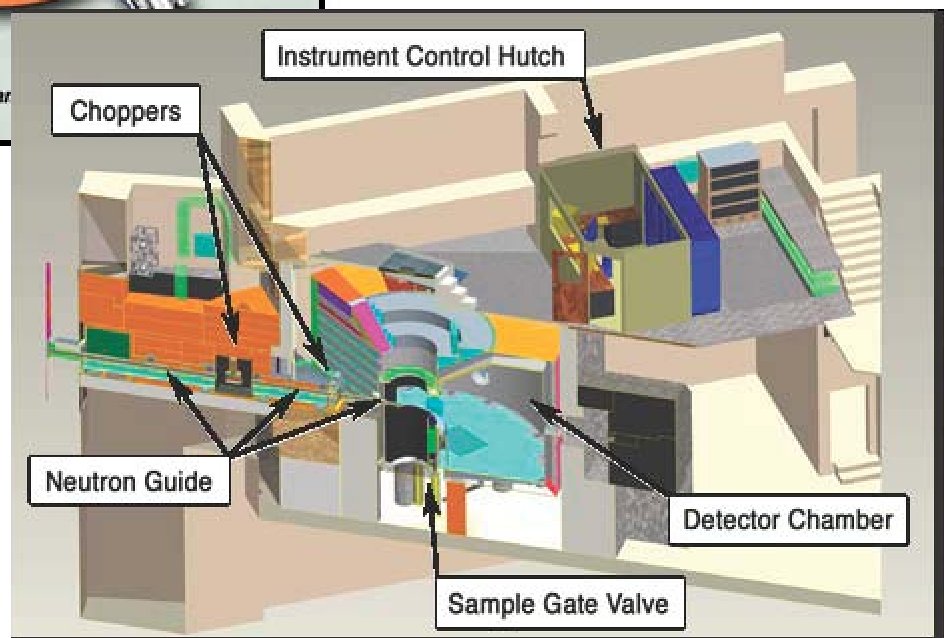
Bragg's Law:
$\lambda = 2d \sin\theta$



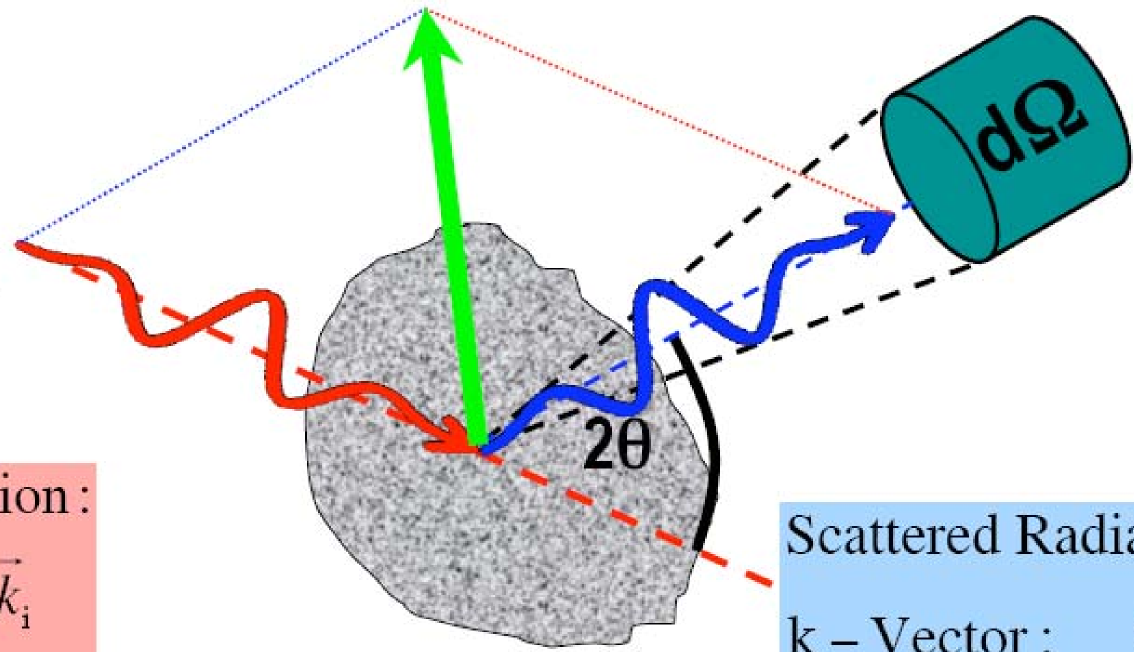
$Q = k_i - k_f$
$\Delta E = (\hbar^2/2m)(k_i^2 - k_f^2)$

Inelastic scattering
$\hbar\omega > 0$ "Energy loss"
$\hbar\omega < 0$ "Energy gain"


Beryllium
Reflector
Cold Source


Instrument Control Hutch
Choppers
Neutron Guide
Detector Chamber
Sample Gate Valve

Scattering Geometry



Incident Radiation:

k – Vector: $\vec{k}_i$

$|\vec{k}_i| = 2\pi / \lambda$

Energy: E_i

Polarization: $\vec{p}_i$

Scattered Radiation:

k – Vector: $\vec{k}_f$

Energy: E_f

Polarization: $\vec{p}_f$

Wavevector Transfer:

$\vec{q} = \vec{k}_f - \vec{k}_i$

Energy Transfer:

$\Delta E = E_f - E_i = \hbar\omega$

Polarization:

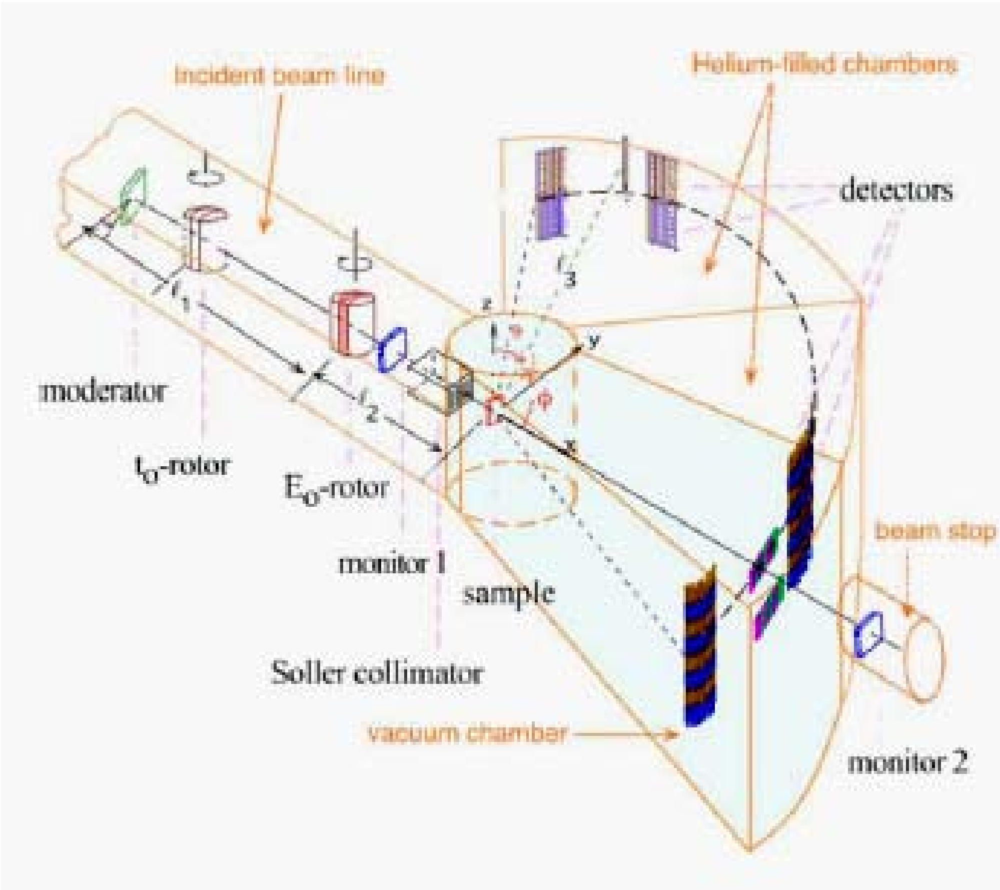
$\vec{p}_i \rightarrow \vec{p}_f$

For X-Rays:

$\Delta E << E_f, E_i$

$\Rightarrow \quad |\vec{q}| = 2k_i \sin(2\theta / 2)$

Wide Angular-Range Chopper Spectrometer (ARCS)



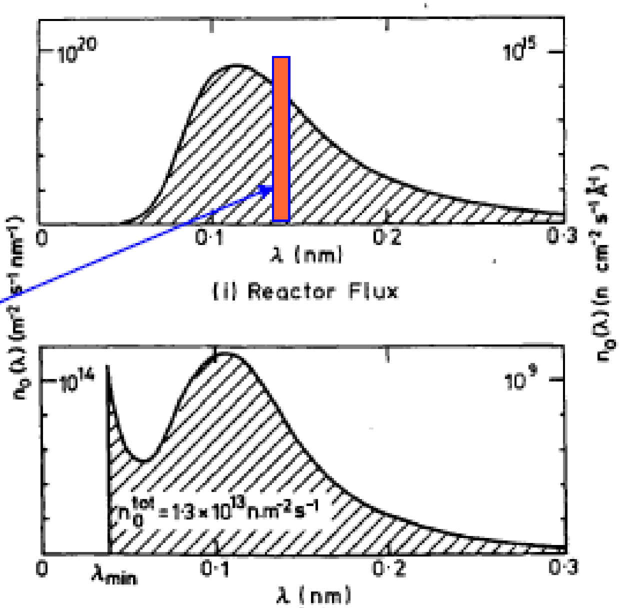
- Primary Flight Path: 11.6m
- Secondary Flight Path: 3m
- Angular range :
  - -30°-150° (Horizontal)
  - -30°-30° (Vertical)
- Incident energy : 10meV-1.5eV
- Energy resolution : 2-5%Ei
- Detectors : Position sensitive
- Supermirror guide
- Oscillating collimator
- Provision for polarization analysis

X-rays, Neutrons and Electrons

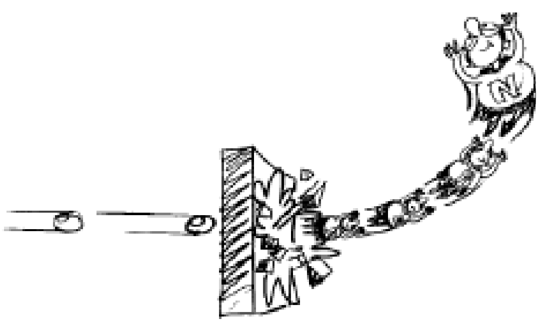
	X-rays	Neutrons	Electrons
	$\lambda = \frac{hc}{E}$	$\lambda = \frac{h}{\sqrt{2m_n E}}$	$\lambda = \frac{h}{\sqrt{2m_e E}}$
Practical Units	$\lambda[\AA] = \frac{12.4}{E[keV]}$	$\lambda[\AA] = \frac{9.08}{\sqrt{E[meV]}}$	$\lambda[\AA] = \frac{12.3}{\sqrt{E[eV]}}$
Energy Range	1-100 keV	10-1000 meV	$10\text{-}10^5$ eV
Wavelength Range [Å]	10-0.1	3-0.3	4-0.04
Penetration Depth	1-100μm	1-50mm	1-100Å

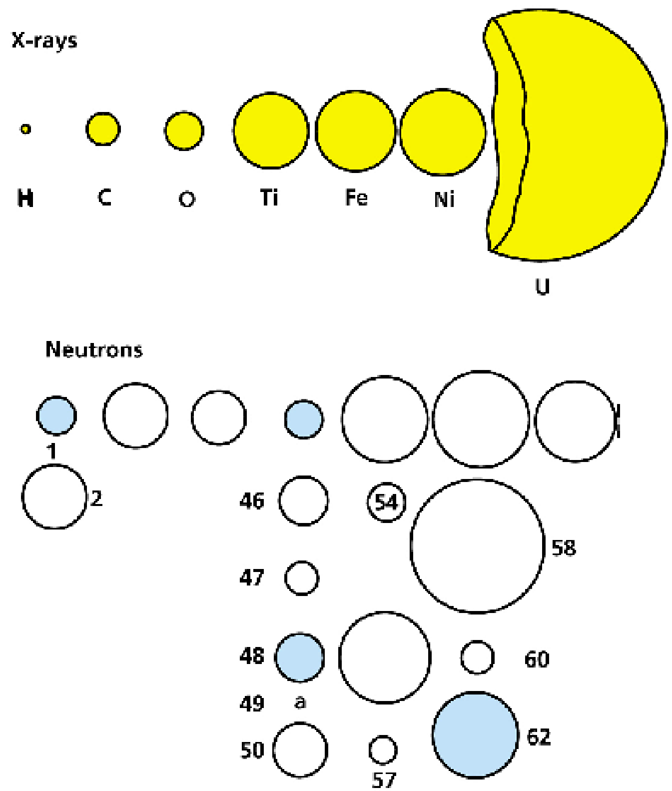
Neutron sources – steady state (Reactors) and pulsed (Spallation)

- Reactor
  - Fission of U^{235} produces neutrons
  - Fission spectrum moderated (slowed down) by either D_2O or H_20 (less good moderator) and neutrons are extracted through beam tubes for spectrometers – fixed wavelength used
- Spallation source
  - High E protons (e.g., 800 MeV) impinge on target (W, Hg or U)
  - Nucleus of target is raised to excited state and subsequent decay produces neutrons (+ γs, neucleons and neutrinos) – 15 – 25 neutrons produced per proton with average E = 55 MeV
  - Neutrons moderated by liquid H, H_20 or methane
  - Spallation sources generally operate in pulse mode – 20 Hz at LANSCE, 60 Hz at new SNS



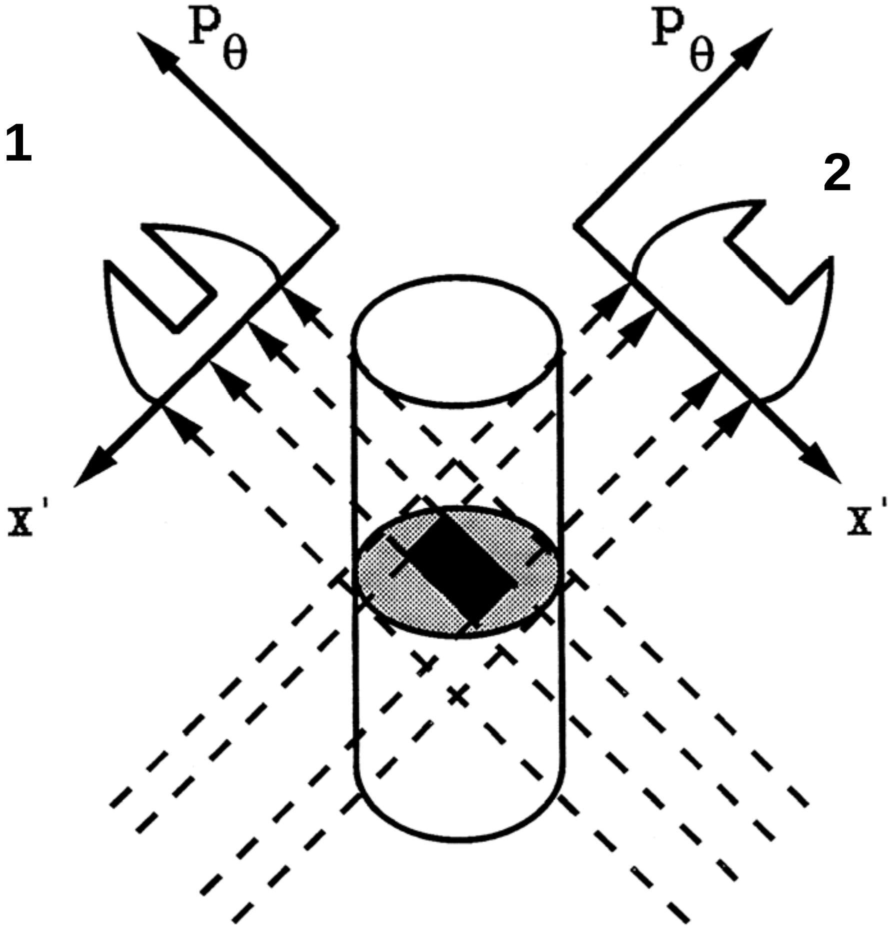
Time of flight is used to sort out wavelengths





X-rays
H
C
O
Ti
Fe
Ni
U
Neutrons
1
2
46
54
58
47
48
60
49
a
50
57
62

How reconstruction works (cartoon)



Along direction 1, the high absorption rectangle makes a spatially narrow but deep "valley" in the absorption profile P_θ.

Along direction 2, the profile P_θ has a spatially wide, but shallow "valley".

At intermediate angles the edges of the valley are less sharp.